Installing and Running CMAQ on discover

Introduction

The Community Multi-scale Air Quality (CMAQ) modeling system has been designed to approach air quality as a whole by including state-of-the-science capabilities for modeling multiple air quality issues, including tropospheric ozone, fine particles, toxics, acid deposition, and visibility degradation. In this way, the development of CMAQ involves the scientific expertise from each of these areas and combines the capabilities to enable a community modeling practice. CMAQ was also designed to have multi-scale capabilities so that separate models were not needed for urban and regional scale air quality modeling.

More information on CMAQ can be obtained at

http://www.cmaq-model.org/

This documentation is intended to help users install the CMAQ package on *discover* using the Fortran Intel compiler and the Intel MPI module.

Obtaining the Code

Obtaining the CMAQ requires the creation of a CMAS account from the link:

http://www.cmascenter.org/register/create_account.cfm

A version of the package is available on *discover* at:

/usr/local/other/CMAQ

where you can obtain the files:

M3MODELS.CMAQv4.6.tar.gz

M3SCRIPTS.CMAQv4.6.tar.gz

Create a Working Directory

```
mkdir myWorkDir
setenv workDir path_to_myWorkDir
```

Now untar the files:

```
cd $workDir
gunzip -c M3MODELS.CMAQv4.6.tar.gz | tar xvf -
```

You will then have the directory CMAQv4.6/. Execute the following commands:

```
cd  CMAQv4.6
gunzip -c M3SCRIPTS.CMAQv4.6.tar.gz | tar xvf -
setenv M3HOME $workDir/CMAQv4.6
setenv M3DATA $M3HOME/data
setenv M3LIB $M3HOME/lib
setenv M3MODEL $M3HOME/models
```

Initial Settings

You need to load modules in order to be able to compile the code:

```
module purge
module load comp/intel-10.1.017 mpi/impi-3.2.011 lib/mkl-10.0.5.025
setenv FC mpiifort
```

In case you have not done so, you will need to set the password-less login on *discover* by following the instructions in:

https://modelingguru.nasa.gov/clearspace/docs/DOC-1112

Required Precompiled Libraries

netCDF

The user needs to provide the netCDF library file *libnetcdf.a*. On *discover* it is available (compatible with the Fortran compiler loaded above) at:

/usr/local/other/netcdf/3.6.2_intel-10.1.013/lib

```
cd $M3LIB
mkdir netCDF netCDF/Linux
cd netCDF/Linux
ln -s /usr/local/other/netcdf/3.6.2_intel-10.1.013/lib/libn* .
```

IOAPI

Step 1

Create a directory (say +IOAPI/+) where you want to install the IOAPI package and go to that directory. The execute the commands:

```
gunzip -c ioapi-3.0.tar.gz | tar
xvf -
setenv BIN Linux2_ia64ifort
mkdir $BIN
cd $BIN
ln -s /usr/local/other/netcdf/3.6.2_intel-10.1.013/lib/libn* .
```

Step 2

In the file Makefile edit BASEDIR and INSTALL and have the following set:

CPLMODE = nocpl # turn off PVM coupling mode

IOAPIDEFS= # for "nocpl"

PVMINCL = /dev/null # for "nocpl"

Step 3

In ioapi/Makefile.nocpl edit BASEDIR and INSTDIR and copy file to ioapi/Makefile.

<u>Step 4</u>

In m3tools/Makefile.nocpl edit BASEDIR and INSTDIR and copy file to m3tools/Makefile.

<u>Step 5</u>

In iotest/Makefile.nocpl edit BASEDIR and copy file to iotest/Makefile.

<u>Step 6</u>

In notcdf/Makefile edit BASEDIR and INSTDIR.

<u>Step 7</u>

Check to see of flags and compilers are set correctly in ioapi/Makeinclude.$BIN

FC = ifort -auto -cm -w90 -w95 -warn notruncated_source

MFLAGS = -traceback

MPFLAGS = -openmp

OMPLIBS = -liomp5 -lpthread

<u>Step 8</u>

Type:

```
make nocpl
```

Copying IOAPI Files to CMAQ Directories

```
cd $M3LIB
mkdir ioapi_3 ioapi_3/ioapi ioapi_3/ioapi/fixed_src ioapi_3/$BIN
```

copy the IOAPI include files (.EXT files) from the directory *IOAPI/ioapi/fixed_src/* to the directory *ioapi_3/ioapi/fixed_src/*.

Copy the library libioapi.a in the directory ioapi_3/$BIN

Compiling CMAQ6

First we want to make the following modifications in the code to allow proper execution. Edit the file

$M3MODEL/CCTM/src/par/par/distr_env.c,v

to change the size of +TEMP_BUF_SIZE* and **CURR_STR_SIZE** to

#define TEMP_BUF_SIZE 20480

#define CURR_STR_SIZE 20480

The following steps are described in

http://www.cmaq-model.org/op_guidance_4.6/html/ch03s03.html

<u>Step 1</u> **Compiling M3BLD**

```
cd $M3HOME/scripts/build
./bldit.m3bld
```

<u>Step 2</u> **Compiling the stenex Libraries**

```
cd $M3HOME/scripts/stenex
```

Edit the file *bldit.se.pgf* to:

(1) **Replace**

set INCL = /share/linux/bin/mpich-ch_p4/include

with

set INCL = .

(2) **Comment out** the line

set FC = /share/linux/pgi/linux86/5.0/bin/pgf90

(3) **Replace**

set FSTD = "-Mfixed -Mextend -c"

with

set FSTD = "-fixed -extend_source 132 -c"

And type:

```
./bldit.se.pgf
```

Edit the file *bldit.se_noop.pgf* to:

(1) **Comment out** the line

set FC = /share/linux/pgi/linux86/5.0/bin/pgf90

(2) **Replace**

set FSTD = "-Mfixed -Mextend -c"

with

set FSTD = "-fixed -extend_source 132 -c"

And type:

```
./bldit.se_noop.pgf
```

Step 3 **Creating the Parallel I/O Library**

```
cd $M3HOME/scripts/pario
```

Edit the file *bldit.pario.pgf* to:

(1) **Replace**

set MPI = /share/linux/bin/mpich-ch_p4/include

with

set MPI = .

(2) **Comment out** the line

set FC = /share/linux/pgi/linux86/5.0/bin/pgf90

(3) **Replace**

set FSTD = "-Mfixed -Mextend -c"

with

set FSTD = "-fixed -extend_source 132 -c"

Step 4 **Compiling JROC**

```
cd $M3HOME/scripts/jproc
```

Edit the file *bldit.jproc.pgf* to:

(1) **Replace**

set FC = /share/linux/pgi/linux86/5.0/bin/pgf90

with

set FC = /usr/local/intel/comp/10.1.017/bin/ifort

(2) **Replace**

set FSTD = "-Mfixed -Mextend"

with

set FSTD = "-fixed -extend_source 132 -openmp"

(3) **Replace**

set LINK_FLAGS = "-Bstatic"

with

set LINK_FLAGS = "-Bstatic -openmp"

(4) **Replace**

set IOAPI = "${M3LIB}/ioapi_3/${BLD_OS}2_x86pg -lioapi"

with

set IOAPI = "${M3LIB}/ioapi_3/${BLD_OS}2_ia64ifort -lioapi"

And type:

```
./bldit.jproc.pgf
```

Step 5 **Compiling ICON and BCON**

```
cd $M3HOME/scripts/icon
```

Edit the file *bldit.icon.pgf* to:

(1) **Replace**

set FC = /share/linux/pgi/linux86/5.0/bin/pgf90

with

set FC = /usr/local/intel/comp/10.1.017/bin/ifort

(2) **Replace**

set FSTD = "-Mfixed -Mextend"

with

set FSTD = "-fixed -extend_source 132 -openmp"

(3) **Replace**

set LINK_FLAGS = "-Bstatic"

with

set LINK_FLAGS = "-Bstatic -openmp"

(4) **Replace**

set IOAPI = "${M3LIB}/ioapi_3/${BLD_OS}2_x86pg -lioapi"

with

set IOAPI = "${M3LIB}/ioapi_3/${BLD_OS}2_ia64ifort -lioapi"

And type:

```
./bldit.icon.pgf
```

```
cd $M3HOME/scripts/bcon
```

Edit the file *bldit.bcon.pgf* to:

(1) **Replace**

set FC = /share/linux/pgi/linux86/5.0/bin/pgf90

with

set FC = /usr/local/intel/comp/10.1.017/bin/ifort

(2) **Replace**

set FSTD = "-Mfixed -Mextend"

with

set FSTD = "-fixed -extend_source 132 -openmp"

(3) **Replace**

set LINK_FLAGS = "-Bstatic"

with

set LINK_FLAGS = "-Bstatic -openmp"

(4) **Replace**

set IOAPI = "${M3LIB}/ioapi_3/${BLD_OS}2_x86pg -lioapi"

with

set IOAPI = "${M3LIB}/ioapi_3/${BLD_OS}2_ia64ifort -lioapi"

And type:

```
./bldit.bcon.pgf
```

Step 6 **Compiling MCIP**

```
cd $M3HOME/scripts/mcip3
```

Edit the file *Makefile* to set:

IOAPI = /discover/nobackup/kouatch/T21820/CMAQv4.6/lib/ioapi_3/Linux2_ia64ifort

NETCDF = /usr/local/other/netcdf/3.6.2_intel-10.1.013

FC = /usr/local/intel/comp/10.1.017/bin/ifort

FFLAGS = -O4 -pc 32 -free -I$(NETCDF)/include

LIBS = -L$(IOAPI) -lioapi -openmp -L$(NETCDF)/lib -lnetcdf

And type:

```
   make
```

Step 7 **Compiling and Running CCTM**

```
cd $M3HOME/scripts/cctm
```

Edit the file *bldit.cctm.pgf* to:

(1) **Replace**

set MPICH = /share/linux/bin/mpich-ch_p4

with

set MPICH =

(2) **Replace**

set FC = /share/linux/pgi/linux86/5.0/bin/pgf90

with

set FC = /usr/local/intel/mpi/3.2.011/bin64/mpiifort

(3) **Replace**

set FSTD = "-Mfixed -Mextend"

with

set FSTD = "-noD -fixed -extend_source 132 -openmp"

(4) **Replace**

set LINK_FLAGS = "-Bstatic"

with

set LINK_FLAGS = "-openmp"

(5) **Replace**

set IOAPI = "${M3LIB}/ioapi_3/${BLD_OS}2_x86pg -lioapi"

with

set IOAPI = "${M3LIB}/ioapi_3/${BLD_OS}2_ia64ifort -lioapi"

(6) **Comment out** the line with "set LIB4"

(7) **Set** Str2 to:

Str2 = (include SUBST_MPICH /usr/local/intel/mpi/3.2.011/include/mpif.h;)

And type:

```
./bldit.cctm.pgf
```

The executable is:

$M3HOME//scripts/cctm/CCTM_e3a

Copy the necessary input data into directory *M3DATA* and edit the file

$M3HOME//scripts/cctm/run.cctm

to include the following (for an 8-processor run) on the top of the file:

#PBS -S /bin/csh

#PBS -N cmaqTest

#PBS -l select=1:ncpus=8:proc=harp

#PBS -l walltime=0:20:00

#PBS -W group_list=yourGroupId

#PBS -j eo

and the following on the bottom of the file (commenting out what is there) for submitting the executable:

time $MPIRUN -np $NPROCS $BASE/$EXEC

Now you are ready to submit the batch script *run.cctm* by typing:

```
qsub run.cctm
```